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Potentials of Gas Laser Components and of Laser Atmospheric-Constituents

FINAL REPORT

we have completed the detailed structural study of a number of complexes of carbon dioxide. The structure of molecular complexes of carbon dioxide may be of considerable importance in developing a better complete understanding of energy transfer processes in the important carbon dioxide laser and especially in our understanding of the earth's (and other planetary) atmosphere.

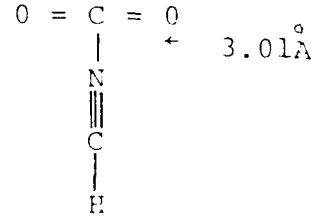
Earlier studies performed under the support of AFOSR produced structural results for the CO_2 HF complex. This together with the study of SCO HF and N_2O HF showed a problem of considerable complexity. The structures of CO_2 HF and SCO HF are linear hydrogen bonded structures with atomic arrangement written. The structure N_2O HF, a species iso-electronic to CO_2 HF, has a highly nonlinear arrangement. The prediction of the geometry of CO_2 complexes is clearly likely to be complicated.

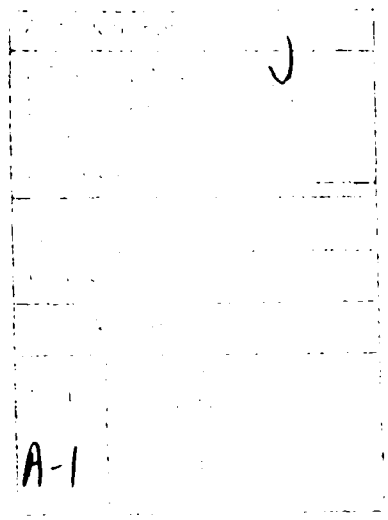
In pursuing the detailed structure of carbon dioxide complexes the system CO_2 HCl (J. Chem. Phys. 77, 4344 (1982)) has been shown to be similar to CO_2 HF. We have recently completed the study of the system HCN CO_2. Although HCN is well known to form hydrogen bonds the structure of this system is not hydrogen bonded. The results of this study are:

	HCN CO_2	DCN CO_2
A	11861.5(18) MHz	12133.1 MHz
B	2226.51(10) MHz	2093.9 MHz
C	1861.60(11) MHz	1764.9 MHz
μ_a	3.2005(60) D	3.2235(55) D
eqQ_N	-4.068(41) MHz	----
τ_{bbbb}	-38 (18) kHz	----
τ_{abab}	-570(475) kHz	----

k_s = .0489 mdyne/Å

R_{cm} = 3.60 Å ; R_{N-C} = 3.01 Å





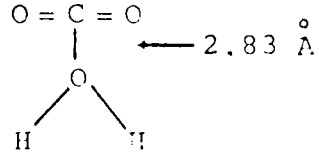
Of great general interest is the complex of CO_2 and H_2O. The importance of this species in the earth's atmosphere is not clear presently. We are in the process of completing the rotational spectrum of the three isotopic species $H_2O\ CO_2$, $D_2O\ CO_2$ and $HDO\ CO_2$. The results at the present stage of research are the rotational constants and electric dipole moment components. These are listed in Table I.

TABLE I

Average Rotational Constant and Electric Dipole Moment for Water Carbon Dioxide Complexes

	H_2OCO_2	D_2OCO_2	$HDOCO_2$
B+C (MHz)	7979.2	7265.7	7608.5
B-C (MHz)	1361.5	1166.4	1254.7
A (MHz)	11374	11236	11348
μ_a(D)	1.849	1.925	1.899

The structure of the complex is linear with structure



The primary uncertainty presently is the knowledge of the barrier hindering the internal rotation about the C-O axis.

Earlier research emphasized complexes of HF. The present research which initiates studies of complexes with H_2O shows that the structural and dynamical behaviour of these two species HF and H_2O can be quite different. In this sense our early optimism that studies of HF binding would likely be adequate for understanding H_2O binding is certainly unwarranted. It is clear that the H_2O systems require much spectroscopic research to place them in a securely understood position. Complete manuscripts on these two problems, CO_2 HCN and CO_2 H_2O are in the process of preparation.

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